

Ferrocene

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|-----------------------------|--|
| Other names: | Bis(«eta»-cyclopentadienyl) iron Bis(cyclopentadienyl)iron Di(«pi»-cyclopentadienyl)iron Di-2,4-cyclopentadien-1-yliron Dicyclopentadienyl iron Ferrotsen Iron dicyclopentadienyl Iron, bis(«eta»5-2,4-cyclopentadien-1-yl)- Iron, bis(«eta»5-cyclopentadienyl) Iron bis(cyclopentadienide) NSC 2033 Catane |
| Inchi: | InChI=1S/2C5H5.Fe/c2*1-2-4-5-3-1;/h2*1-5H; |
| InchiKey: | DFRHTHSZMBROSH-UHFFFAOYSA-N |
| Formula: | C10H10Fe |
| SMILES: | C12C3C4C5C1[Fe]23451678C2C1C6C7C28 |
| Mol. weight [g/mol]: | 186.03 |
| CAS: | 102-54-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|--------|--------------|
| affp | 863.60 | kJ/mol | NIST Webbook |
| basg | 841.30 | kJ/mol | NIST Webbook |
| chs | -5891.50 ± 4.20 | kJ/mol | NIST Webbook |
| chs | -5877.70 ± 5.00 | kJ/mol | NIST Webbook |
| chs | -5905.30 ± 1.70 | kJ/mol | NIST Webbook |
| hf | 228.60 ± 4.60 | kJ/mol | NIST Webbook |
| hf | 231.70 ± 4.10 | kJ/mol | NIST Webbook |
| hf | 242.40 ± 2.50 | kJ/mol | NIST Webbook |
| hf | 214.80 ± 5.30 | kJ/mol | NIST Webbook |
| hfs | 154.90 ± 4.50 | kJ/mol | NIST Webbook |
| hfs | 168.70 ± 2.30 | kJ/mol | NIST Webbook |
| hfs | 141.10 ± 5.20 | kJ/mol | NIST Webbook |
| hfs | 158.00 ± 4.00 | kJ/mol | NIST Webbook |
| h vap | 64.70 ± 0.40 | kJ/mol | NIST Webbook |
| ie | 7.10 | eV | NIST Webbook |
| ie | 6.82 | eV | NIST Webbook |

| | | | |
|----|---------------|---------|--------------|
| ie | 6.61 ± 0.08 | eV | NIST Webbook |
| ie | 6.90 ± 0.20 | eV | NIST Webbook |
| ie | 6.60 | eV | NIST Webbook |
| ie | 6.75 ± 0.01 | eV | NIST Webbook |
| ie | 7.00 | eV | NIST Webbook |
| ie | 6.72 | eV | NIST Webbook |
| ie | 6.75 ± 0.25 | eV | NIST Webbook |
| ie | 6.78 ± 0.05 | eV | NIST Webbook |
| ie | 6.90 ± 0.10 | eV | NIST Webbook |
| ie | 7.20 ± 0.10 | eV | NIST Webbook |
| ie | 6.97 | eV | NIST Webbook |
| ie | 6.99 | eV | NIST Webbook |
| ie | 6.90 | eV | NIST Webbook |
| ie | 6.86 | eV | NIST Webbook |
| ie | 6.90 | eV | NIST Webbook |
| ie | 6.88 | eV | NIST Webbook |
| ie | 6.88 | eV | NIST Webbook |
| ie | 6.71 ± 0.08 | eV | NIST Webbook |
| ie | 6.90 ± 0.10 | eV | NIST Webbook |
| ss | 216.20 | J/mol×K | NIST Webbook |
| ss | 211.85 | J/mol×K | NIST Webbook |
| tb | 519.00 ± 1.00 | K | NIST Webbook |
| tf | 446.00 ± 0.50 | K | NIST Webbook |
| tf | 447.00 | K | NIST Webbook |
| tf | 451.30 ± 0.50 | K | NIST Webbook |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------------|---------|-----------------|--------------|
| cps | 195.90 | J/mol×K | 298.16 | NIST Webbook |
| cps | 189.56 | J/mol×K | 298.15 | NIST Webbook |
| cps | 192.50 | J/mol×K | 298.00 | NIST Webbook |
| cps | 131.00 | J/mol×K | 200.00 | NIST Webbook |
| hfust | 17.78 | kJ/mol | 448.20 | NIST Webbook |
| hfust | 17.49 | kJ/mol | 447.60 | NIST Webbook |
| hfust | 17.80 | kJ/mol | 448.50 | NIST Webbook |
| hsubt | 70.50 | kJ/mol | 406.00 | NIST Webbook |
| hsubt | 70.00 ± 2.00 | kJ/mol | 363.00 | NIST Webbook |
| hsubt | 84.00 ± 2.00 | kJ/mol | 420.00 | NIST Webbook |
| hsubt | 83.30 | kJ/mol | 345.00 | NIST Webbook |
| hsubt | 73.20 ± 1.90 | kJ/mol | 301.00 | NIST Webbook |

| | | | | |
|-------|--------------|--------|--------|--------------|
| hsubt | 72.60 ± 0.10 | kJ/mol | 313.00 | NIST Webbook |
| hsubt | 73.10 ± 1.40 | kJ/mol | 333.00 | NIST Webbook |
| hsubt | 72.50 ± 1.00 | kJ/mol | 296.00 | NIST Webbook |
| hsubt | 72.10 ± 0.40 | kJ/mol | 293.50 | NIST Webbook |
| hsubt | 64.60 | kJ/mol | 397.00 | NIST Webbook |
| hvapt | 47.30 | kJ/mol | 456.00 | NIST Webbook |
| hvapt | 44.70 | kJ/mol | 561.50 | NIST Webbook |
| hvapt | 49.80 | kJ/mol | 487.00 | NIST Webbook |
| hvapt | 47.30 | kJ/mol | 489.50 | NIST Webbook |

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C102545&Units=SI>

Legend

| | |
|---------------|--|
| affp: | Proton affinity |
| basg: | Gas basicity |
| chs: | Standard solid enthalpy of combustion |
| cps: | Solid phase heat capacity |
| hf: | Enthalpy of formation at standard conditions |
| hfs: | Solid phase enthalpy of formation at standard conditions |
| hfust: | Enthalpy of fusion at a given temperature |
| hsubt: | Enthalpy of sublimation at a given temperature |
| hvap: | Enthalpy of vaporization at standard conditions |
| hvapt: | Enthalpy of vaporization at a given temperature |
| ie: | Ionization energy |
| ss: | Solid phase molar entropy at standard conditions |
| tb: | Normal Boiling Point Temperature |
| tf: | Normal melting (fusion) point |

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